

Analytical and Numerical Demonstration of How the Drude Dispersive Model Satisfies Nernst's Theorem for the Casimir Entropy

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Abstract. In view of the current discussion on the subject, an effort is made to show very accurately both analytically and numerically how the Drude dispersion model, assuming the relaxation is nonzero at zero temperature (which is the case when impurities are present), gives consistent results for the Casimir free energy at low temperatures. Specifically, we find that the free energy consists essentially of two terms, one leading term proportional to T^2 , and a next term proportional to $T^{5/2}$. Both these terms give rise to zero Casimir entropy as $T \rightarrow 0$, thus in accordance with Nernst's theorem.

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1. Introduction

The thermodynamic consistency of the expression for the Casimir pressure at finite temperature T is of considerable current interest. The problem gets accentuated at low T , where according to Nernst's theorem $S = -\partial F/\partial T \rightarrow 0$ when $T \rightarrow 0$. Here S is the entropy and F the free energy per unit surface area. We shall consider the standard Casimir configuration, namely two semi-infinite identical metallic media separated by a vacuum gap of width a . The media are assumed nonmagnetic with a frequency-dependent relative permittivity $\varepsilon(\omega)$. The two surfaces lying at $z = 0$ and $z = a$ are taken to be perfectly planar and of infinite extent. A sketch of the setup is given in figure 1.

The present work is closely related to our recent paper [1] in particular, and also to our earlier papers on the thermal Casimir effect [2, 3, 4, 5, 6].

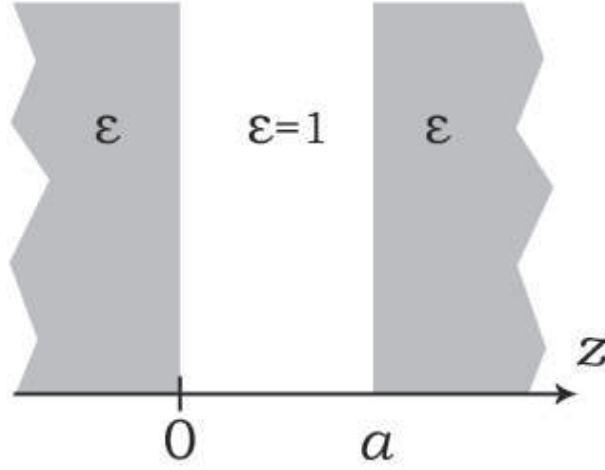


Figure 1. Sketch of the geometry

We start from the Lifshitz formula:

$$\beta F = \frac{1}{2\pi} \sum'_{m=0} \int_{\zeta_m/c}^{\infty} \left[\ln(1 - Ae^{-2qa}) + \ln(1 - Be^{-2qa}) \right] q \, dq, \quad (1)$$

where

$$A = \left(\frac{s - \varepsilon p}{s + \varepsilon p} \right)^2 \quad (\text{TM mode}) \quad (2a)$$

$$B = \left(\frac{s - p}{s + p} \right)^2 \quad (\text{TE mode}) \quad (2b)$$

$$\zeta_m = \frac{2\pi k}{\hbar} mT, \quad \beta = 1/kT \quad (2c)$$

$$s = \sqrt{\varepsilon - 1 + p^2}, \quad p = \frac{qc}{\zeta_m}. \quad (2d)$$

Here ζ_m are the Matsubara frequencies, s and p are the Lifshitz variables, and the prime on the summation sign means that the case $m = 0$ is to be taken with half weight.

The appropriate dispersion relation to use is the Drude relation

$$\varepsilon(i\zeta) = 1 + \frac{\omega_p^2}{\zeta(\zeta + \nu)}, \quad (3)$$

where $\omega = i\zeta$, ω_p being the plasma frequency, and ν the relaxation frequency. The plasma wavelength is $\lambda_p = 2\pi c/\omega_p$. Our motivation for adopting the form (3) is that it agrees well with permittivity measurements (performed at room temperature). In the case of gold,

$$\omega_p = 9.03 \text{ eV}, \quad \nu = 34.5 \text{ meV}, \quad \lambda_p = 137.4 \text{ nm}. \quad (4)$$

The Drude relation is good for $\zeta < 2 \times 10^{15}$ rad/s. For higher ζ , the relation gives too low values for the permittivity (cf. figure 1 in [6]). Actually, the numerical input data

we used were taken directly from tabulated data along the imaginary frequency axis, $\varepsilon(i\zeta)$ for $\zeta > 0$ (courtesy of Astrid Lambrecht). These data cover 7 decades:

$$1.5 \times 10^{11} < \zeta < 1.5 \times 10^{18} \text{ rad/s.} \quad (5)$$

For $\zeta < 1.5 \times 10^{11}$ values for $\varepsilon(i\zeta)$ are obtained from (3) by extrapolation, but by our numerical evaluations only the $m = 0$ value fell within this region.

As mentioned, the permittivity measurements are made at room temperature. For definiteness, we shall in the following use the room-temperature value $\nu = 34.5 \text{ meV}$ already given in (4), although we expect that at very low temperatures the true value of ν is actually lower - cf. the recent discussion on this point by Klimchitskaya and Mostepanenko [7]. This fact will change our results quantitatively, but not qualitatively. In particular, it will not change our main conclusion regarding the validity of the Nernst theorem when $T \rightarrow 0$.

Let us emphasize the main assumption underlying our calculations: *We assume ν to possess a nonzero value, however small, at any fixed temperature including $T = 0$.*

The assumed constancy of ν might be questioned, as the Bloch-Grüneisen law predicts that ν depends on T as (cf. Appendix D in [6])

$$\nu(T) \propto T^5, \quad T \rightarrow 0. \quad (6)$$

Such a relationship is not followed in practice, however, since there are always impurities which give rise to nonzero resistivity and so nonzero relaxation frequency at zero temperature [8]. In practice, therefore, our assumption above is always satisfied. The important point is that the relationship

$$\zeta^2[\varepsilon(i\zeta) - 1] \rightarrow 0, \quad \zeta \rightarrow 0 \quad (7)$$

is always satisfied. It implies that the zero-frequency TE mode does not contribute to the Casimir force. The first to emphasize this kind of behaviour were Boström and Sernelius [9], and the issue was discussed in detail in [6]. There are several other papers arguing along similar lines. Thus Jancovici and Šamaj [10] and Buenzli and Martin [11] considered the classical plasma of free charges in the high-temperature limit, where only zero frequency contributes, and they found the linear dependence in T in the Casimir force to be reduced by a factor of 2 from the behaviour of an *ideal* metal (the IM model).

To illustrate the magnitude of the Drude thermal correction to the Casimir pressure, we give in Table 1 some calculated values, in mPa. It should be noted that if T increases from 300 K to 350 K, we find that

- (i) if $a = 0.2 \text{ } \mu\text{m}$, the Casimir pressure diminishes by 0.4%;
- (ii) if $a = 2.0 \text{ } \mu\text{m}$, the Casimir pressure diminishes by 3.7%.

The optimum gap width in connection with Casimir thermal corrections thus seem to lie around $a = 2 \text{ } \mu\text{m}$.

An argument that has been put forward against the Drude relation is that by omitting the zero frequency TE term one gets a term linear in T in the free energy. Such a term would lead to a finite entropy at $T = 0$ and so come into conflict with Nernst's theorem. There are several recent papers arguing along these lines, written

Table 1. The Casimir pressure (in mPa) between Au-Au plates versus gap width a , when $T = \{1, 300, 350\}$ K. Data extracted from Ref. [3].

$a/\mu\text{m}$	$T = 1$ K	$T = 300$ K	$T = 350$ K
0.2	508.2	497.8	495.7
0.5	16.56	15.49	15.30
1.0	1.143	0.9852	0.9590
2.0	7.549×10^{-2}	5.550×10^{-2}	5.344×10^{-2}
3.0	1.520×10^{-2}	1.033×10^{-2}	1.049×10^{-2}
4.0	4.858×10^{-3}	3.481×10^{-3}	3.804×10^{-3}

from somewhat different perspectives [7, 12, 13, 14, 15, 16, 17], and it is argued there that for such lattices the Drude model violates the Nernst theorem. Perfect crystal lattices, without impurities at all, are considered in these papers. It is argued therein that for thermodynamical consistency, relaxation due to electron-phonon scattering present at finite temperature should be neglected, and the use of the plasma dispersion relation

$$\varepsilon(i\zeta) = 1 + \frac{\omega_p^2}{\zeta^2}, \quad (8)$$

or a generalized version thereof is presented. The relation (8) corresponds to setting $\nu = 0$ in (3), such that (8) does *not* satisfy the condition (7). The plasma relation leads to quite a small temperature dependence in the Casimir force (correction $\propto T^4$) in contrast to the distinct and almost linear decay with the Drude relation. Actually, the Drude theory in the limit $\nu \rightarrow 0$ preserves entropy $S = 0$ at $T = 0$, but S changes more and more abruptly at $T = 0$ the smaller ν is.

In the following we intend to show very accurately, both analytically and numerically, how the Drude relation with $\nu \neq 0$ leads to results that are in full agreement with the Nernst theorem.

2. Analytical approach

We start from the Drude model assuming some constant value for ν , and consider in the following only Matsubara frequencies that are relatively small, $\zeta (\equiv \zeta_m) \ll \nu$. These frequencies are the crucial ones for the behavior in the $T \rightarrow 0$ limit. It is always possible to consider these frequencies when ν , as mentioned above, is finite. Then,

$$\varepsilon(i\zeta) = \frac{\omega_p^2}{\zeta(\zeta + \nu)} \approx \frac{D}{\zeta}, \quad D = \frac{\omega_p^2}{\nu}. \quad (9)$$

We consider only the TE mode, which is the mode of main interest. Replace q by x :

$$x^2 = \frac{q^2 c^2}{(\varepsilon - 1)\zeta^2} = \frac{q^2 c^2}{D\zeta}, \quad \zeta \ll \nu. \quad (10)$$

Then the TE mode coefficient (2b) becomes

$$B = (\sqrt{1 + x^2} - x)^4, \quad (11)$$

and the TE part of the free energy can be written

$$\beta F^{TE} = C \sum_{m=0}^{\infty} g(m), \quad (12)$$

where

$$g(m) = m \int_{\sqrt{\zeta/D}}^{\infty} x \ln \left[1 - B \exp \left(-\frac{2a}{c} \sqrt{D\zeta} x \right) \right] dx. \quad (13)$$

Now invoke the Euler-Maclaurin formula:

$$\sum_{m=0}^{\infty} g(m) = \int_0^{\infty} g(u) du - \frac{1}{12} g'(0) + \frac{1}{720} g'''(0) - \dots \quad (14)$$

One then finds that

$$g'(0) = \int_0^{\infty} x \ln(1 - B) dx = -\frac{1}{4} (2 \ln 2 - 1). \quad (15)$$

And thereby one gets

$$\Delta F^{TE} = \frac{C}{48\beta} (2 \ln 2 - 1) = \frac{1}{48} \frac{\omega_p^2}{c^2 \hbar \nu} (kT)^2 (2 \ln 2 - 1), \quad (16)$$

valid for $T \ll 0.01$ K. This result was first given by Milton at the QFEXT03 workshop [5].

Including the leading correction (Euler-Maclaurin summation starting at $m = 1$ instead of at zero), one gets [1]

$$\Delta F^{TE} = \frac{C}{\beta} \left[-\frac{1}{12} g'(0) \right] \left[1 + 0.204 \frac{3a\sqrt{2\pi C}}{12g'(0)} + \dots \right]. \quad (17)$$

For gold plates, with $a = 1 \mu\text{m}$

$$\Delta F^{TE} = C_1 T^2 [1 - C_2 T^{1/2} + \dots], \quad (18)$$

with

$$C_1 = 5.81 \times 10^{-13} \text{ (J/m}^2 \text{ K}^2\text{)}, \quad C_2 = 3.03 \text{ K}^{-1/2}. \quad (19)$$

In order to avoid negative values for T slightly larger than 0.1 K, it is convenient to introduce the Padé approximant form

$$\Delta F_{th}^{TE} = \frac{C_1 T^2}{1 + C_2 T^{1/2}}. \quad (20)$$

This is equivalent to (18) with respect to the first two terms. Results (18) - (20) were first obtained in Ref. [1].

3. Numerical calculations

In the numerical calculations we assume two gold plates, with $a = 1 \mu\text{m}$. All dispersive data needed are in the experimentally known region given by (5) above. As mentioned, the only place where there is a need to use Drude relation (3) explicitly, is when $m = 0$. Actually, it is immaterial whether we use the experimental Lambrecht data (5) or the Drude relation directly. Thus figure 4 is calculated with the use of the Drude relation

for all frequencies, but it turns out that a practically identical figure (with some noise because of lower accuracy) is obtained if we use Lambrecht's data.

At $T = 0$ the free energy is calculated numerically as a double integral rather than a sum of integrals, using a two-dimensional version of Simpson's method with adaptive quadrature.

As for the TM mode, it is known that for ideal or nonideal metals the temperature correction for this mode behaves as T^4 . Thus, it is a smaller correction than the T^2 and $T^{5/2}$ corrections associated with the TE mode. We repeat that the dependence of ν on temperature is neglected, and that we employ the room-temperature values for ν given in (4).

The vanishing of the zero-frequency mode is connected with the behaviour of the coefficient B at vanishing frequency. To illuminate this point, we show in figure 2 both coefficients A and B as a function of imaginary frequency and transverse momentum k_\perp for an interface between gold and vacuum. In part (c) of the figure, we see how $B \rightarrow 0$ when $\zeta \rightarrow 0$ for $k_\perp \neq 0$, whereas A in figure 2(a) for the TM mode equals 1 for all k_\perp when $\zeta \rightarrow 0$.

By direct numerical integration and lengthy summations independent of the analytical derivations made in the previous section, we obtain the free energy numerically. Figure 3 shows the free energy versus temperature up to 800 K, while the inset shows details of the parabolic shape close to $T = 0$. The figure shows the decrease of the magnitude of the free energy and thus also the related decrease of the Casimir force up to a certain temperature. The inset shows how the slope is horizontal at $T = 0$, as predicted. Thus the entropy at $T = 0$ is zero, in accordance with Nernst's theorem.

4. A more accurate test

Now, there are always uncertainties connected with numerical calculations. It is possible to make a much more accurate and sensitive test of the behaviour near $T = 0$ in the following way. Define the quantity R as the relative difference between the temperature-dependent theoretical free energy $\Delta F_{\text{th}}^{\text{TE}}$, and the temperature-dependent numerical free energy $\Delta F_{\text{num}}^{\text{TE}}$:

$$R = \frac{\Delta F_{\text{th}}^{\text{TE}} - \Delta F_{\text{num}}^{\text{TE}}}{\Delta F_{\text{th}}^{\text{TE}}} \quad (21)$$

Assume for $\Delta F_{\text{th}}^{\text{TE}}$ the Padé approximant form (20), and assume for $\Delta F_{\text{num}}^{\text{TE}}$ the expansion

$$\Delta F_{\text{num}}^{\text{TE}} = D_1(T^2 - D_2T^{5/2} + D_3T^3 + \dots) \quad (22)$$

with calculated values for the coefficients D_1 , D_2 and D_3 . Then,

$$R = \frac{C_1 - D_1}{C_1} + \frac{D_1}{C_1}(D_2 - C_2)T^{1/2} + \frac{D_1}{C_1}(C_2D_2 - D_3)T + \dots \quad (23)$$

If $C_1 = D_1$ and $C_2 = D_2$:

$$R(T = 0) = 0, \quad R \propto T, \quad T \rightarrow 0. \quad (24)$$

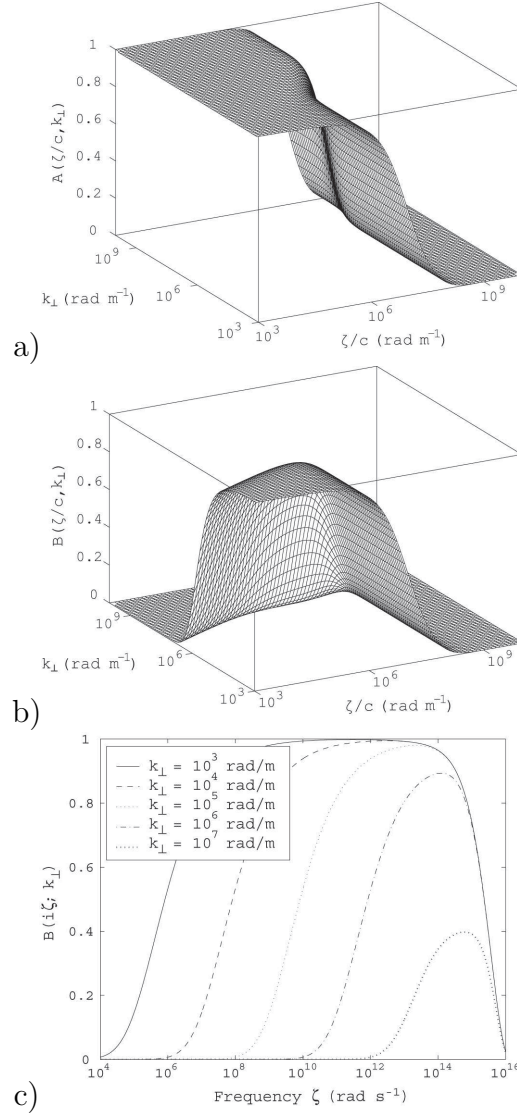


Figure 2. Squared reflection coefficients A and B of the metal interfaces for the TM and TE modes, as a function of ζ/c and the transverse momentum k_{\perp} . a) A for the TM mode, b) B for the TE mode, c) B for k_{\perp} and ζ close to zero.

Calculated values of R are plotted in figure 4. We see that R , when extrapolated, approaches zero linearly with a finite slope. This demonstrates the accuracy of the T^2 and $T^{5/2}$ terms in the free energy.

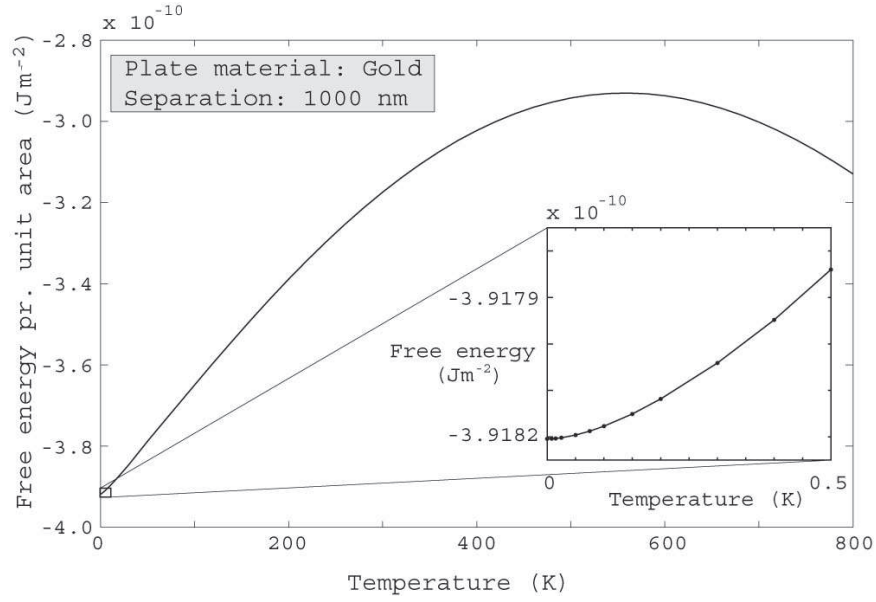


Figure 3. Numerical evaluation of the free energy (1) between two gold half-spaces as a function of temperature. The inset gives details for low T .

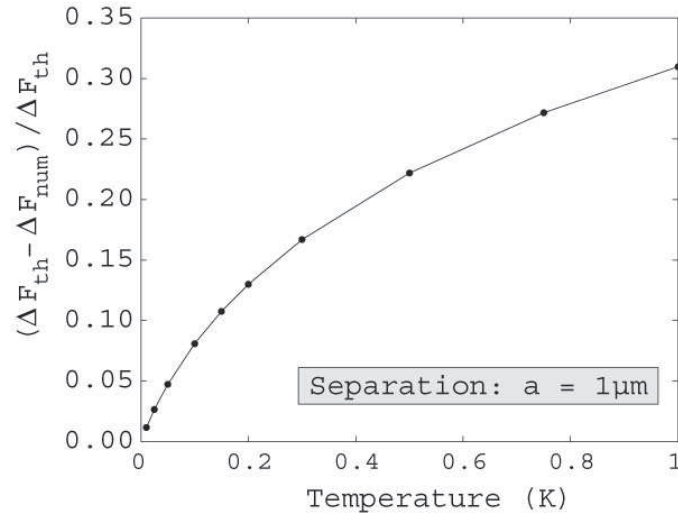


Figure 4. Plot of the ratio R defined in (21).

5. Alternative derivation by expansion of $g(m)$

It may be of interest to mention that, as a variant of the analytic approach, the dependence of the free energy on T near $T = 0$ can be found by means of complex integration. Start from the TE expression

$$\beta F = C \sum_{m=0}^{\infty} \int_{\sqrt{\xi/D}}^{\infty} x \ln(1 - Be^{-\alpha x}) dx, \quad (25)$$

where

$$C = \frac{\omega_p^2}{\beta \hbar \nu c^2}, \quad \alpha = 2a\sqrt{2\pi C m}, \quad (26)$$

and expand the logarithm,

$$\beta F^{TE} = -C \sum_{m=1}^{\infty} m \int_0^{\infty} x \sum_{n=1}^{\infty} B^n e^{-n\alpha x} dx. \quad (27)$$

Now use the formula

$$e^{-n\alpha x} = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} ds (n\alpha x)^{-s} \Gamma(s), \quad 4 > c > 0 \quad (28)$$

and sum over m ,

$$\sum_{m=1}^{\infty} m^{1-s/2} = \zeta\left(\frac{s}{2} - 1\right). \quad (29)$$

Here ζ denotes the Riemann zeta function. Distorting the contour so as to encircle the poles of the Γ function at $s = 0, -1, \dots$ then yields the same result (18) as above.

6. Summary and further remarks

The main point in our analysis has been to show both analytically and numerically that the Drude dispersion relation (3) does not run into conflict with basic thermodynamics, as long as $\nu \neq 0$ at $T = 0$. As we have seen, quite an accurate analysis is needed for this purpose. If we instead had argued in a more crude way, simply setting the TE coefficient $B_m = 0$ for $m = 0$ and keeping all the other coefficients A_m and B_m equal to 1 as in the modified ideal metal model (MIM), then we would have broken Nernst's theorem. This issue has been discussed at length in Refs. [6] and [18].

Whether the Drude predictions for the Casimir force are correct or not is to be decided upon from experiments. A difficulty here is the inherent uncertainty of theoretical predictions due to the relatively large spread of published data for the dielectric permittivity for typical metals such as Au - cf., for instance, the recent discussions on this point by Pirozhenko *et al.* [19] and Munday and Capasso [20]. The experiment with the highest precision [15, 16] apparently is in disagreement with the Drude model, or any model satisfying (7). It has also been suggested that there are large thermal effects due to surface roughness [21]. We might note that the 1% precision in the dynamic measurement made by the Purdue group [15, 16] is not matched by the 3% accuracy of the very recent dynamic experiment reported in Ref. [22]. Our main concern in the present paper, however, has been to discuss the consistency of this theory. We wish to point out that it would be quite strange if the Drude relation, proved to be representing permittivity measurements with great accuracy, should turn out to be inapplicable to explain Casimir force measurements. Let us also mention here that an interesting discussion about the thermal Casimir effect and the Johnson noise has recently been given by Bimonte [23], as a possible theoretical explanation for the discrepancy with experiment.

The basic assumption for our analysis ought to be re-emphasized. We assumed the relaxation frequency ν to be a *finite quantity*, for any value of T . One might here raise the question: what happens if the metal is a perfect crystal, with no impurities at all? In such a case $\nu(T = 0) = 0$, and the formalism above becomes inapplicable. (In this we have an opinion different from the definitive claim of a violation of the Nernst theorem given in Refs. [17, 15], for example. See also Ref. [24].) On basis of the calculation above, we can thus make no firm statement about the validity of the Nernst theorem in this special case.

We ought to mention, though, that on physical grounds there are conceptual difficulties in simply setting $\nu = 0$ in the dispersion relation:

(i) It would yield a contribution to the Casimir force from the zero frequency TE mode. This mode is however not a solution of Maxwell's equations and should therefore not occur. (A more detailed discussion can be found in Ref. [6], and in Sect. III in Ref. [25].)

(ii) Introducing a zero TE mode for perfect crystals would imply that such a medium would behave differently from a real metal when taking the limit $\nu = 0$. This would create a discontinuity in behaviour that we find unphysical.

There are additional physical effects that we have not taken into account above:

(1) One such effect is *spatial dispersion* [26], implying that the wave vector \mathbf{k} is present in the dispersion relation. Then $\varepsilon = \varepsilon(\omega, k)$ would become finite for finite k . Only the special case $\varepsilon(0, 0)$ would be infinite, and it would not appear natural that this "measure zero" case should yield a finite contribution to the Casimir force.‡

(2) Another effect that could have been taken into account is the *anomalous skin effect* [28, 29]. This effect occurs when the mean free path in the metal becomes much larger than the field penetration depth near $T = 0$. Again, no contribution to the Casimir force is found from the zero TE mode, and the Nernst theorem is satisfied.

Finally, we refer to the very recent microscopic theory of the Casimir force at large separations, i.e. the classical limit, using statistical mechanics [30] - cf. also [31] and further references therein. These authors make use of a joint functional representation of both matter and field, enabling them to integrate out the field degrees of freedom entirely. Important in our context is that they find the TE modes not to contribute in this regime, and that the Casimir surface pressure is

$$P = -\frac{\zeta(3)kT}{8\pi a^3}, \quad a \rightarrow \infty. \quad (30)$$

This is precisely as predicted by the Drude model in the same limit. This conclusion is further supported by Svetovoy's recent demonstration [32] of the cancellation between TE evanescent wave (EW) and propagating wave (PW) contributions for large distances, yielding Eq. (30), while at short distances the TE EW dominates for the force between two metal plates or between a metal plate and a dielectric plate, resulting in a linear temperature term in the force.

‡ It could be mentioned here that the contrary view has been expressed in Ref. [27].

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